Precursor and neutral loss scans in a single ion trap and application to planetary exploration

Completed Technology Project (2017 - 2021)

Project Introduction

Precursor and neutral loss scans are general survey methods in tandem mass spectrometry that allow for the detection of molecules with similar functional groups. For example, a neutral loss scan can target hydroxylated compounds, and a precursor scan can target glycosylated molecules. Despite their utility, precursor and neutral loss scans are typically reserved for large, complex, and power-hungry multi-analyzer instruments (e.g. the triple quadrupole mass spectrometer). However, such instruments are not suitable for planetary missions due to their size and high power consumption as well as their requirement for relatively high vacuum conditions. Ion traps, on the other hand, are ideally suited for these missions due to their lower power consumption, versatility, high pressure tolerance, high sensitivity and selectivity, and capabilities for single analyzer tandem mass spectrometry. Fitting under TABS element 8.3.3 In-situ (other) instrumentation, we propose to implement precursor and neutral loss scans in a single quadrupole ion trap. Using dual orthogonal ac waveforms for precursor ion excitation and product ion ejection, we will develop methods for precursor and neutral loss scanning in both benchtop and miniature ion trap mass spectrometers. Both techniques require precise control of the trapping radiofrequency (rf) field as well as nonlinear ac frequency scanning that must be calculated using a program that will be written in-house. Precursor ion fragmentation will be controlled by mass-selectively exciting the entire precursor ion population successively at the same Mathieu q value, set by the excitation ac frequency. Simultaneously, as they are produced, product ions corresponding to a particular mass-to-charge ratio (which corresponds to a particular molecular structure) will be ejected from the trap and detected, preserving the mass information encoded in the excitation of the precursor ions. The performance of this technique will be evaluated on several fronts: precursor ion fragmentation efficiency, product ion ejection efficiency, sensitivity, limits of detection, spectral resolution, and unintended 'ghost peaks'. This technology has great benefits for planetary exploration. Survey scans will enable the discovery of molecules in different molecular classes using minimal sample and a single data-independent mass scan. This contrasts with current data-dependent methods which require more time, sample volume, several ion injections into the trap, or multiple ion traps. Furthermore, the developments proposed here would provide further evidence for the utility of single ion traps as small, power-efficient, and capable organic molecule analyzers in planetary exploration instrument suites. All of the known tandem mass spectrometry scans (precursor, neutral loss, and product ion scans) would be at the disposal of the ion trap, increasing its utility for analysis of small organic molecules. Such a set of scans would be beneficial for answering the fundamental questions about the origin of life, which may be answered in part by detecting small organic molecules on comets and planets.

Anticipated Benefits

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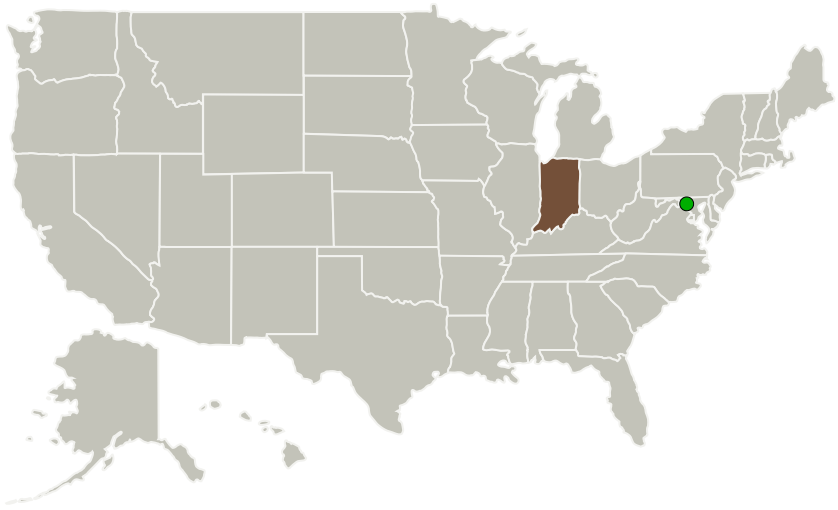
Primary U.S. Work Locations and Key Partners



Organizations Performing Work	Role	Type	Location
Purdue University-Main Campus	Lead Organization	Academia	West Lafayette, Indiana
Goddard Space Flight Center(GSFC)	Supporting Organization	NASA Center	Greenbelt, Maryland

Primary U.S. Work Locations
Indiana

Organizational Responsibility

Responsible Mission Directorate:

Space Technology Mission Directorate (STMD)

Lead Organization:

Purdue University-Main Campus

Responsible Program:

Space Technology Research Grants

Project Management

Program Director:

Claudia M Meyer

Program Manager:

Hung D Nguyen

Principal Investigator:

Robert G Cooks

Co-Investigator:

Dalton T Snyder

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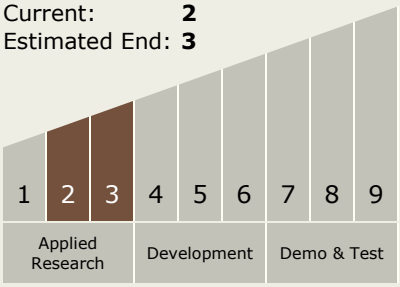
Technology Maturity (TRL)

Start: **2**
Current: **2**
Estimated End: **3**



Technology Areas

Primary:

- TX08 Sensors and Instruments
  - TX08.3 In-Situ Instruments and Sensors
    - TX08.3.1 Field and Particle Detectors

Target Destinations

Mars, Others Inside the Solar System